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Phase Transitions and the Mass of the Visible Universe

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Recent results on QCD thermodynamics are presented. The nature of the T>0 transition is determined, which turns out to be an analytic cross-over. The absolute scale for this transition is calculated. In order to approach the continuum limit four different sets of lattice spacings were used with temporal extensions N_t=4, 6, 8 and 10 (they correspond to lattice spacings a∼0.3, 0.2, 0.15 and 0.12 fm).

1 Introduction

One of the most fundamental fields of all science is the physics of elementary particles. We are looking for the smallest building blocks of nature. We would like to understand their interactions. Since everything is built up from these particles we hope that the knowledge on the physics of the building blocks leads to the understanding of more complex systems. Experimentalists are looking for different particles and interactions, which are then put into a consistent framework by theorists, who have to solve the equations, too. The most popular experimental way to gain information is to collide a few particles and look what happened. Many more particles were participating in these high energy processes in the early Universe (Big Bang) or are participating in present day heavy ion experiments (Little Bang). Note, that for both cases the baryonic densities are much smaller than the typical hadronic scales (and can be treated as zero).

At temperatures around $T \approx 200$ MeV a transition happened, which is related to the spontaneous breaking of the chiral symmetry of QCD. The nature of the QCD transition affects our understanding of the Universe's evolution (see ref.[1] and references therein). In a strong first-order phase transition the quark–gluon plasma supercools before droplets of hadron gas are formed. These droplets grow, collide and merge, during which gravitational waves could be produced[2]. Baryon-enriched nuggets could remain between the bubbles, contributing to dark matter. The hadronic phase is the initial condition for nucleosynthesis, so inhomogeneities in this phase could have a strong effect on nucleosynthesis. As the first-order phase transition weakens, these effects become less pronounced. Since about 99% of the mass of the visible Universe is generated during this transition, it is of extreme importance to understand its details. As we will see our calculations provide strong evidence that the QCD transition is a cross-over and thus the above scenarios – and many others – are ruled out. In addition we determine the absolute scale of this transition in physical units. The determination of the absolute scale pins down the temperature and time scale in the early Universe and has a huge impact on present and future heavy ion experiments.

Quantum chromodynamics (QCD) is the theory of the strong interaction, explaining (for example) the binding of three almost massless quarks into a much heavier proton or neutron – and thus most of the mass of the visible Universe. The strong interaction is

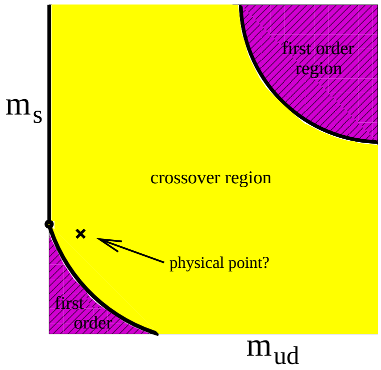

Figure 1. The phase diagram of QCD on the hypothetical light quark mass versus strange quark mass plane. Thick lines correspond to second order phase transitions, the purple regions represent first order phase transitions and the yellow region represents an analytic cross-over.

responsible for the energy producing processes in the sun or in nuclear reactors. The standard model of particle physics predicts a QCD-related transition. At low T, the dominant degrees of freedom are colourless bound states of hadrons (such as protons and pions). However, QCD is asymptotically free, meaning that at high energies or temperatures the interaction gets weaker and weaker[3,4], causing hadrons to break up. This behaviour underlies the predicted cosmological transition between the low T hadronic phase and a high T quark–gluon plasma phase (for simplicity, we use the word 'phase' to characterize regions with different dominant degrees of freedom). Despite enormous theoretical effort, the nature of this $T > 0$ QCD transition (that is, first-order, second-order or analytic cross-over) remained ambiguous. The reason for that is the extreme complication when one tries to solve the equations of QCD. Since they describe the strong interaction they are strongly coupled equations, which seem to be impossible to be solved analytically. The only known systematic technique which could give a final answer is lattice QCD.

QCD is a generalised version of quantum electrodynamics (QED). The Euclidean Lagrangian with gauge coupling g and with a quark mass of m can be written as $\mathcal{L}=-1/(2g^2)\mathrm{Tr}F_{\mu\nu}F_{\mu\nu}+\bar{\psi}\gamma_\mu(\partial_\mu+A_\mu+\mathrm{m})\psi$, where $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu+[A_\mu,A_\nu]$. In QED the gauge field A_μ is a simple real field, whereas in QCD it is a 3×3 matrix. Consequently the commutator in $F_{\mu\nu}$ vanishes for QED, but it does not vanish in QCD. The ψ fields also have an additional "colour" index in QCD, which runs from 1 to 3. Different types of quarks are represented by fermionic fields with different m. The action S is defined as the four-volume integral of $\mathcal{L}$. The basic quantity we determine is the the partition function Z, which is the sum of the Boltzmann factors $\exp(-S)$ for all field configurations. Partial derivatives of Z with respect to m give rise to the order parameters we studied here.

Lattice QCD (c.f.[5]) discretises the above Lagrangian on a four-dimensional lattice and extrapolates the results to vanishing lattice spacing ($a \longrightarrow 0$). A convenient way to carry out this discretisation is to put the fermionic variables on the sites of the lattice, whereas the gauge fields are treated as 3×3 matrices connecting these sites. In this sense, lattice QCD is a classical four-dimensional statistical physics system. One important difference compared to three dimensional systems is that T is determined by the additional, Euclidean

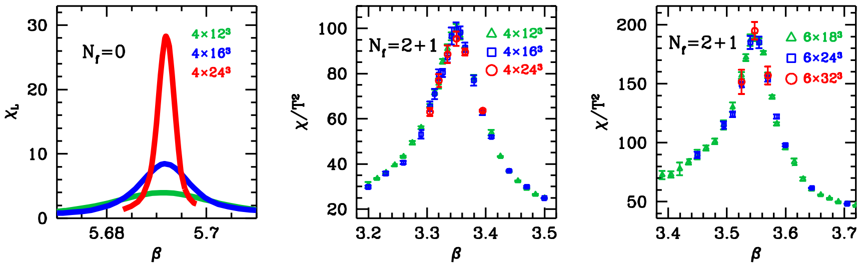

Figure 2. The V dependence of the susceptibility peaks for pure SU(3) gauge theory (Polyakov susceptibility, left panel) and for full QCD (chiral susceptibility on N_t= 4 and 6 lattices, middle and right panels, respectively).

time extension (N_t): T=1/($N_t a$). Keeping T fixed (such as T_c, the transition temperature) one can reduce a and approach the continuum limit by increasing N_t.

2 The Nature of the QCD Transition

The standard picture for the QCD phase diagram on the light quark mass (m_{ud}) versus strange quark mass (m_s) plane is shown by Fig. 1. It contains two regions at small and at large quark masses, for which the $T > 0$ QCD transition is of first order. Between them one finds a cross-over region, for which the $T > 0$ QCD transition is an analytic one. The first order transition regions and the cross-over region are separated by lines, which correspond to second order phase transitions. The location of the physical point (thus the nature of the QCD transition) was a priori unknown.

There are lattice results for the nature of the transition (for the two most popular lattice formulations see refs[6,7]), although they have unknown systematical errors. We emphasize that from the lattice point of view two "ingredients" are necessary to eliminate the systematical errors.

The first ingredient is to use physical quark masses. Owing to the computational costs this is a great challenge in lattice QCD. Previous analyses used computationally less demanding non-physically large quark masses. However, these choices have limited relevance. The order of the transition depends on the quark mass. For example, in three-flavour QCD for vanishing quark masses the transition is of first-order. For intermediate masses it is a cross-over. For infinitely heavy quark masses the transition is again first-order. For questions concerning the restoration of chiral symmetry (such as the order of the transition), a controlled extrapolation from larger quark masses (such as chiral perturbation theory) is unavailable, and so the physical quark masses should be used directly.

The second ingredient is to remove the uncertainty associated with the lattice discretization. These errors disappear in the continuum limit; however, they strongly influence the results at non-vanishing lattice spacing. E.g. in three-flavour unimproved staggered QCD, using a lattice spacing of about 0.28 fm, the first-order and the cross-over regions are separated by a pseudoscalar mass of $m_{\pi,c}$≈300 MeV. Studying the same three-flavour theory with the same lattice spacing, but with an improved p4 action (which has different

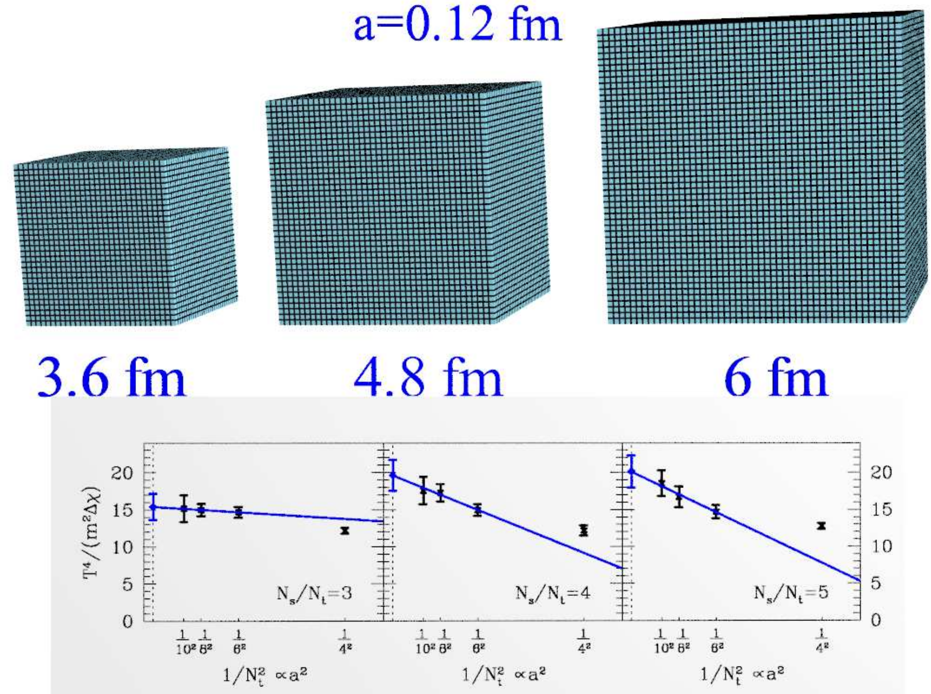

Figure 3. The upper pictures show three different physical V-s with our finest discretization. The lower plots show the dimensionless quantity $T^4/(m^2\Delta\chi)$ as a function of a^2 and their continuum extrapolated values. No V dependence is observed.

discretization errors) we obtain $m_{\pi,c}\approx$70 MeV. In the first approximation, a pseudoscalar mass of 140 MeV (which corresponds to the numerical value of the physical pion mass) would be in the first-order transition region, whereas using the second approximation, it would be in the cross-over region. The different discretisation uncertainties are solely responsible for these qualitatively different results[8]. Therefore, the proper approach is to use physical quark masses, and to extrapolate to vanishing lattice spacings.

Our work eliminates both of the above uncertainties[9].

We will study the finite size scaling of the lattice chiral susceptibilities $\chi(N_s, N_t)$=$\partial^2/(\partial m_{ud}^2)(T/V)\cdot \log Z$, where m_{ud} is the mass of the light u,d quarks and N_s is the spatial extension. This susceptibility shows a pronounced peak around T_c. For a real phase transition the height of the susceptibility peak increases and the width of the peak decreases when we increase the volume (V). For a first-order phase transition the finite size scaling is determined by the geometric dimension, the height is proportional to V, and the width is proportional to $1/V$. Such an example can be seen on the left panel of Fig. 2. In the pure SU(3) gauge theory –QCD with no fermions– the transition is known to be of first order. Thus, the characteristic increase of the analogous susceptibility can be seen. For a second-order transition the singular behaviour is given by some power of V, defined by the critical exponents. The picture would be completely different for an analytic

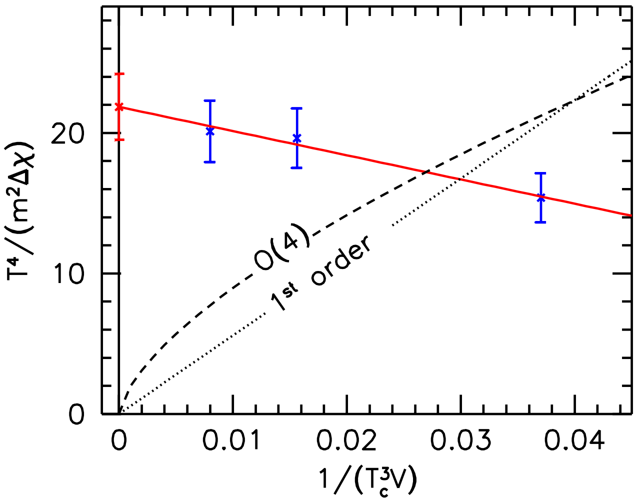

Figure 4. Continuum extrapolated susceptibilities $T^4/(m^2\Delta\chi)$ as a function of $1/(T_c^3V)$. For true phase transitions the infinite V extrapolation should be consistent with zero, whereas for an analytic cross-over the infinite V extrapolation gives a non-vanishing value. The continuum-extrapolated susceptibilities show no phase-transition-like volume dependence, though V changes by a factor of five. The $V\to\infty$ extrapolated value is 22(2) which is 11σ away from zero. For illustration, we fit the expected asymptotic behaviour for first-order and O(4) (second order) phase transitions shown by dotted and dashed lines, which results in chance probabilities of 10^{-19} (7×10^{-13}), respectively.

cross-over. There would be no singular behaviour and the susceptibility peak does not get sharper when we increase V; instead, its height and width will be V independent for large V. Quite interestingly this behaviour is observed for full QCD, the susceptibility peaks are almost V independent (see the middle and right panels of Fig. 2 for the susceptibilities for the light quarks for $N_t = 4$ and 6, for which we used aspect ratios $r = N_s/N_t$ ranging from 3 to 6 and 3 to 5, respectively).

Unfortunately, these curves do not say much about the continuum behaviour of the theory. In principle a phenomenon as unfortunate as that in the three-flavour theory could occur[8], in which the reduction of the discretization effects changed the nature of the transition for a pseudoscalar mass of ≈140 MeV.

In order to clarify this issue (which is a genuine $T > 0$ effect) we subtract the T= 0 susceptibility and study only the difference between $T \neq 0$ and T= 0 at different lattice spacings. This leads to $m^2\Delta\chi$, which we study. To give a continuum result for the nature of the transition we carry out a finite size scaling analysis of the dimensionless quantity $T^4/(m^2\Delta\chi)$ directly in the continuum limit. For this study we need the height of the susceptibility peaks in the continuum limit for fixed physical V. The continuum extrapolations are done using four different lattice spacings. The V-s at different lattice spacings are fixed in units of T_c, and thus VT_c^3=3^3,4^3 and 5^3 were chosen. Fig. 3 shows one typical discretization of our different physical sizes and the continuum extrapolation for these three volumes. N_t=4 results are off, N_t=6,8 and 10 show a good $a^2\propto1/N_t^2$ scaling.

Having obtained the continuum values for $T^4/(m^2\Delta\chi)$ at fixed physical V-s, we study the finite V scaling of the results. Fig. 4 shows our final results. The V dependence shows

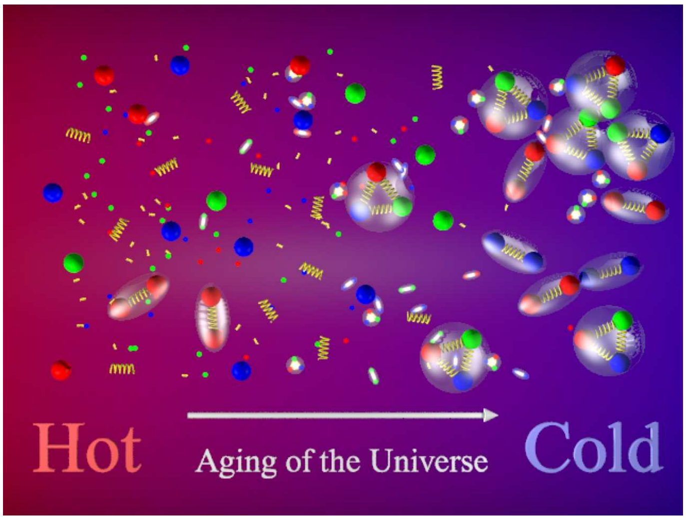

Figure 5. A schematic view of the transition between the quark-gluon plasma and the hadronic phase. Free quarks and gluons are confined to hadrons as the Universe cools. The transition is smooth, no singularity appears.

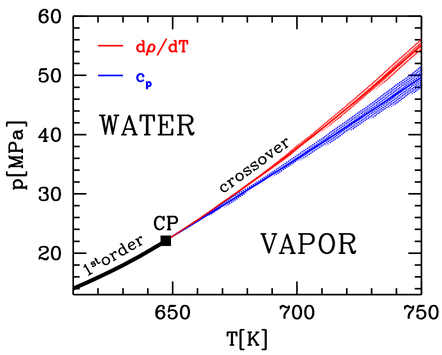

Figure 6. The water-vapour phase diagram.

that there is no true phase transition but only an analytic cross-over in QCD.

Thus, no droplet formation happened, the quark-gluon plasma went through smoothly to a hadronic phase. This smooth transition is shown as a cartoon on Fig. 5.

3 The Transition Temperature

An analytic cross-over, like the QCD transition has no unique T_c. A particularly nice example for that is the water-vapour transition (c.f. Fig. 6). Up to about 650 K the transition is a first order one, which ends at a second order critical point. For a first or second order phase transition the different observables (such as density or heat capacity) have their singularity (a jump or an infinitely high peak) at the same pressure. However, at even

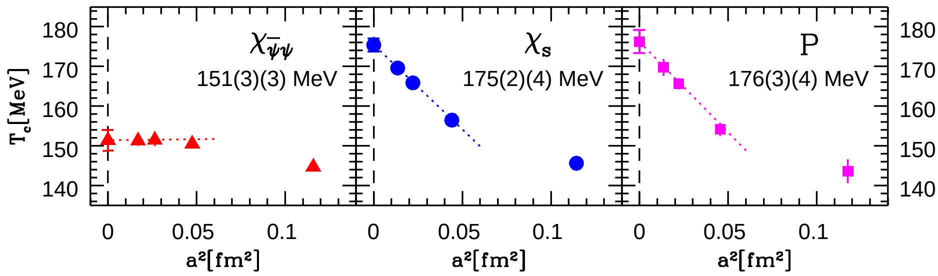

Figure 7. Continuum limits of T_c obtained from the renormalized chiral susceptibility ($m^2\Delta\chi_{\bar\psi\psi}/T^4$), strange quark number susceptibility (χ_s/T^2) and renormalized Polyakov-loop (P_R).

higher T-s the transition is an analytic cross-over, for which the most singular points are different. The blue curve shows the peak of the heat capacity and the red one the inflection point of the density. Clearly, these T_c-s are different, which is a characteristic feature of an analytic transition (cross-over). In QCD we will study the chiral and the quark number susceptibilities and the Polyakov loop. Usually they give different T_c values, but there is nothing wrong with it. As was illustrated by the water-vapour transition it is a physical ambiguity, related to the analytic behaviour of the transition. There is another, non-physical, ambiguity. If we used different observables (particularly at large lattice spacings) to set the lattice spacings we obtain different overall scales. They lead to different T_c values. This ambiguity disappears in the continuum limit.

According to our experiences, at finite lattice spacings, the best choice is the kaon decay constant f_k. It is known experimentally (in contrast to the characteristics of the static potential), thus no intermediate calculation with unknown systematic errors is involved. Furthermore, it can be measured on the lattice quite precisely. The continuum extrapolated T_c values obtained[10] for different quantities are shown on Fig. 7.

There is a surprising several sigma effect. The remnant of the chiral transition happens at a quite different T than that of the deconfining transition. It is a robust effect, since the Polyakov transition region is quite off the χ-peak, and the χ-peak is far from the inflection point of the Polyakov loop. This quite large difference is also related to the fact that the transition is fairly broad. The widths are around 30-40 MeV.

One can set the overall scale by r_0 (it is defined by the static potential between a quark and an antiquark $dV/dr^2 \cdot r_0^2$=1.65). On coarse lattices different choices might lead to ambiguities for the T_c, which is illustrated for our data on Fig. 8. Using only N_t=4 and 6 the continuum extrapolated T_c-s are quite different if one took r_0 or f_K to determine the overall scale. This inconsistency indicates, that these lattice spacings are not yet in the scaling region (a similar ambiguity is obtained by using the p4 action of[11]). Having N_t=4,6,8 and 10 results this ambiguity disappears (as usual N_t=4 is off), these lattice spacings are already in the scaling region (at least within our accuracy). This phenomenon is not surprising. At large a-s the scale cannot be determined unambiguously. This underlines the importance of the continuum limit we carried out.

The ambiguity related to the inconsistent continuum limit is unphysical, and it is resolved as we approach the continuum limit (c.f. Fig. 8). The differences between the T_c

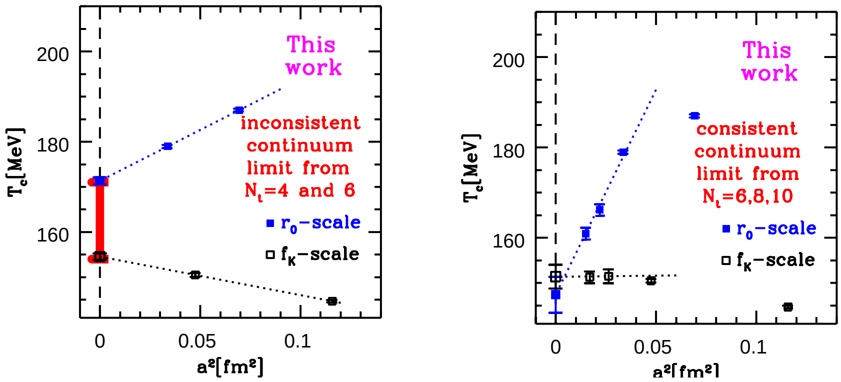

Figure 8. Continuum extrapolations based on N_t=4 and 6 (left panel: inconsistent continuum limit) and using N_t=6,8 and 10 (right panel: consistent continuum limit).

values for different observables are physical, this is a consequence of the cross-over nature of the QCD transition.

4 Summary

The nature of the QCD transition was determined, which turned out to be an analytic cross-over. This result excludes most cosmic relic scenarios. The transition temperature was determined for several observables. Since the transition is a broad one, there is a 30-40 MeV difference between the T_c values defined by different observables.

Acknowledgments

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References

1. D. J. Schwarz, Annalen Phys. **12** (2003) 220 [arXiv:astro-ph/0303574].
2. E. Witten, Phys. Rev. D **30**, 272 (1984).
3. D. J. Gross and F. Wilczek, Phys. Rev. Lett. **30**, 1343 (1973).
4. H. D. Politzer, Phys. Rev. Lett. **30** (1973) 1346.
5. I. Montvay and G. Munster, “Quantum fields on a lattice,” *Cambridge, UK: Univ. Pr. (1994) 491 p.*
6. F. R. Brown *et al.*, Phys. Rev. Lett. **65**, 2491 (1990).
7. A. Ali Khan *et al.* [CP-PACS Collaboration], Phys. Rev. D **63**, 034502 (2001) [arXiv:hep-lat/0008011].
8. F. Karsch et al., Nucl. Phys. Proc. Suppl. **129** (2004) 614 [arXiv:hep-lat/0309116].
9. Y. Aoki, G. Endrodi, Z. Fodor, S. D. Katz and K. K. Szabo, Nature **443** (2006) 675.
10. Y. Aoki, Z. Fodor, S. D. Katz and K. K. Szabo, Phys. Lett. B **643** (2006) 46.
11. M. Cheng et al., Phys. Rev. D **74**, 054507 (2006) [arXiv:hep-lat/0608013].